A model for nanocrystalline diamond growth

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Growth mechanisms for ultrananocrystalline diamond grown in hydrogen-poor argon plasmas are different from conventional CVD growth based on methyl radials. We propose a model that can account for very high renucleation rates necessary to produce diamond with grain sizes in the nanometer scale. The model is based on the calculation of stable adsorbates and transition states for reactions of C_2 with diamond surfaces calculated using electronic structure methods. The nonempirical model invokes transition state theory to calculate reaction rates from the energies and barriers. Resulting renucleation rates and grain sizes provide a mechanism for nanocrystalline diamond growth in the absence of hydrogen. The temperature dependence of renucleation rate as a function of the C_2 density in the plasma was obtained from the model. It shows that a grain size reaches its maximal value at the temperatures of about 800 °C. A comparison of the computed results with available experimental data is provided and further predictions are discussed.

Keywords

diamond growth, nucleation, transition state theory